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Coarse-Grained Modeling of Mixtures of Charged Macroions¹ JUN KYUNG CHUNG, ALAN R. DENTON, Department of Physics, North Dakota State University — In suspensions of charged macroions, such as charge-stabilized colloids and polyelectrolyte microgels, the electrostatic interactions between macroions are relatively easily controlled by changing the sizes and charges of the macroions, as well as the concentration of salt. This tunability of interactions can be exploited to stabilize various structures that self-assemble under appropriate conditions. In this talk, a statistical mechanical coarse-graining approach to modeling effective electrostatic interactions in mixtures of charged spherical macroions will be discussed. Taking effective interactions as input, we perform molecular dynamics simulations to calculate pair distribution functions of binary mixtures of charged colloids. For highly charged macroions, incorporating charge renormalization is found to be important. Using thermodynamic perturbation theory, we also analyze phase behavior and explore the possibility of a demixing instability as a function of size and charge asymmetry.

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Alan Denton North Dakota State University

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